1. Notation: $E(A) = \langle A \rangle$. Then $E(A) = \sum_{i=1,2} A(i)P(i) = (h_1 - h_2)/(h_1 + h_2)$, $E(A^2) = \sum_i A^2(i)P(i) = 1$.
Fluctuation is $V(A) = E[(A - E(A))^2] = E(A^2) - 2[E(A)]^2 + [E(A)]^2 = E(A^2) - [E(A)]^2 = \frac{4h_1h_2}{(h_1+h_2)^2}$.
Dispersion is $\Delta_A = \sqrt{V(A)}/E(A) = 2\sqrt{h_1h_2}/(h_1 + h_2)$.
For $h_1/h_2 \to \infty$, $V(A) \simeq 4h_2/h_1$, $\Delta_A \simeq \sqrt{V(A)}$.

2. Let $w = e^{2i\pi/n}$, $w^n = 1$, $A_l = \mathbf{Re}\, w^l$.
  a) $E(A) = \frac{1}{n}\mathbf{Re}\sum_{l=1}^{n} w^l = \frac{1}{n}\mathbf{Re}\sum_{l=0}^{n-1} w^l = \frac{1}{n}\mathbf{Re}\frac{1-w^n}{1-w} = 0$.
  b) $2A_l^2 = \mathbf{Re}(1+w^{2l})$, so $2E(A^2) = n+\frac{1}{n}\mathbf{Re}\sum_{l=1}^{n}(w^2)^l$. We distinguish two cases: if $n = 2, w^2 = 1, E(A^2) = 2 = n$; if $n > 2, w^2 \neq 1, E(A^2) = n/2$ by the argument given in a).
  c) The system has circular symmetry.

3. Let $(P_{+,-})_n$ be the probabilities of finding the system in states $+, -$ at time $t_n = n\Delta t$. We have the following process:

$$\begin{bmatrix} P_+ \\ P_- \end{bmatrix}_n = \begin{bmatrix} P(+|+) & P(+|-) \\ P(-|+) & P(-|-) \end{bmatrix} \begin{bmatrix} P_+ \\ P_- \end{bmatrix}_{n-1}, \tag{1}$$

where $P(\sigma|\mu)$ is the probability of finding the system at t_n in the state σ, given it was in the state μ at time t_{n-1}. This is simply the law of total probability.
  Since $\sum_\sigma P(\sigma|\mu) = 1$ for any μ, and from $P(+|-) = \alpha(1 + H)/2, P(-|+) = \alpha(1 - H)/2$, we can write

$$v_n = Kv_{n-1}, \tag{2}$$

where $v_n = \begin{bmatrix} P_+ \\ P_- \end{bmatrix}_n$ and

$$K = \begin{bmatrix} \frac{1+a}{2} & \frac{1-b}{2} \\ \frac{1-a}{2} & \frac{1+b}{2} \end{bmatrix}, \tag{3}$$

and $a = 1 - \alpha(1 + H), b = 1 - \alpha(1 - H)$. Denote by v_0 the probabilities for the initial state (they depend on the initial state preparation process) and obtain the solution

$$v_n = K^n v_0, \tag{4}$$

  To compute K^n, write $K = J + B/2$, where

$$J = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}, \quad B = \begin{bmatrix} a & -b \\ -a & b \end{bmatrix} \tag{5}$$

and derive the following properties:

$$J^2 = J, \quad J \cdot B = 0_{2\times 2}, \quad B^2 = (a+b)B \tag{6}$$

It is now easy to obtain $K^n = J + (\frac{a+b}{2})^{n-1}B/2$ by iteration.

Now assume that the initial probabilities are known,

$$v_0 = \begin{bmatrix} u \\ d \end{bmatrix}, \tag{7}$$

with $u + d = 1$. Then

$$v_n = \begin{bmatrix} 1/2 \\ 1/2 \end{bmatrix} + \left(\frac{a+b}{2}\right)^{n-1} \begin{bmatrix} (au - bd)/2 \\ (bd - au)/2 \end{bmatrix}, \tag{8}$$

so the spin average is $E(\sigma)_n = (au - bd)(\frac{a+b}{2})^{n-1}$.

The average over N measurements becomes

$$\overline{E(\sigma)} = \frac{1}{N}\sum_{n=1}^{N} E(\sigma)_n = (au - bd)\frac{\sum_{n=1}^{N}(\frac{a+b}{2})^{n-1}}{N} \tag{9}$$

We have $(a+b)/2 = 1 - \alpha, au - bd = (1-\alpha)(u-d) + \alpha H$, so we get:

$$\overline{E(\sigma)} = \frac{(1-\alpha)(u-d) + \alpha H}{N\alpha}[1 - (1-\alpha)^N]. \tag{10}$$

Clearly, $\lim_{N\to\infty} \overline{E(\sigma)} = 0$. The case $\alpha \to 0$ (zero temperature) is subtle, because it leads to a symmetry breaking mechanism.

4. Saddle point expansion of the integral $(\lambda \gg 1, f'(a) = 0)$

$$\int dt e^{\lambda f(t)} \simeq e^{\lambda f(a)} \sqrt{\frac{\pi}{\lambda}} \sum_{n=0}^{\infty} \frac{(2n)!c_{2n}}{4^n n! \lambda^n}, \tag{11}$$

where $\frac{dg(\tau)}{d\tau} = \sum_{n=0}^{\infty} c_n \tau^n$, and $t = g(\sqrt{f(a) - f(t)})$.

We obtain

$$n! = \int dx x^n e^{-x} = n^{n+1}\int dt e^{-nt + n\ln t} = n\left(\frac{n}{e}\right)^n \int dt e^{-n[t-1-\ln t]} = \sqrt{\pi n}\left(\frac{n}{e}\right)^n \sum_{n=0}^{\infty} \frac{(2n)!c_{2n}}{4^n n! \lambda^n}, \tag{12}$$

where $\frac{dg(\tau)}{d\tau} = \sum_{n=0}^{\infty} cn\tau^n$, and $t = g(\sqrt{t-1-\ln t})$. Thus, $\frac{dg(\tau)}{d\tau} = \frac{dt}{d\sqrt{t-1-\ln t}} = \sum_{n=0}^{\infty} c_n(\sqrt{t-1-\ln t})^n$.
Iterating this identity twice, we obtain $c_0 = \sqrt{2}, c_2 = c_0/12$, so

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$$n! \simeq \sqrt{2\pi n} \left(\frac{n}{e}\right)^n \left[1 + \frac{1}{12n} + O(n^{-2})\right]. \tag{13}$$

Relative error at $n = 15$ is $\frac{1}{180}$.

5. The sum of N independent random variables X_n identically distributed with probabilities $P(1) = p, P(0) = 1 - p$ is a random variable distributed binomially, with N states and parameter p, $X = \sum_{n=1}^{N} X_n$. The magnetization is zero if $X = N/2$ (half of spins up, half down), so $P(M = 0) = \frac{N!}{((N/2)!)^2}[p(1-p)]^{N/2}$.

For $p = 1/2$ (configurations equally likely), we get $P(M = 0) = \frac{N!}{2^N((N/2)!)^2}$. For large N, Stirling's formula gives $P(0) \simeq \sqrt{\frac{2}{\pi N}}$.

<center>Physics 352

Spring 2003

Problem Set 2

Solutions</center>

6. Use the equations of motion $p' = -kx, \quad x' = p/m$ to obtain $H' = pp'/m + kxx' = 0 \rightarrow H = \text{const.}$ and $kx^2/2 = -xp'/2 = px'/2 - (px)'/2 = p^2/2m - (px)'/2$. Therefore, $\overline{kx^2/2} = \overline{p^2/2m} - \overline{(px)'/2} = \overline{p^2/2m}$ since $\overline{f'} = \lim_{\Delta t \to \infty} \int_{\Delta t} f'(t)dt = 0$ for any bounded function $f(t)$. We conclude that $\overline{kx^2/2} = H/2$.

The microcanonical distribution can be expressed as $kx^2/2 + p^2/2m = H$, so we parametrize $kx^2/2 = H\cos(\theta), \quad p^2/2m = H\sin(\theta), \quad \theta \in [0, 2\pi]$. Then $\langle kx^2/2 \rangle = H\frac{1}{2\pi}\int_0^{2\pi}\cos^2(\theta)d\theta = H/2 = \overline{kx^2/2}$.

7. Introduce the notation $z_k = p_k + i\omega_k x_k, \quad k = 1, 2$. Then the Poisson brakets read $\{z_k, z_l\} = 0, \{z_k, \overline{z}_l\} = 2i\omega_k \delta_{k,l}$. We also have $H = |z_1|^2 + |z_2|^2$, so the solutions to the equations of motions are $z_k = |z_k|e^{i\omega_k t} = \sqrt{|\Phi_k|}e^{i\omega_k t + \phi_k}, \quad k = 1, 2$, where ϕ_k are constant phases fixed by initial conditions.

If $\omega_2 = n\omega_1$, we have the invariant $\Phi_3 = Re\{z_1\overline{z_2}^{\frac{1}{n}}\} = Re\{\Phi_1\Phi_2^{\frac{1}{n}}e^{i(\phi_1 - \phi_2/n)}e^{2\pi ir/n}\}, \quad r = \overline{0, n-1}$, with n branches. For $n = 2$, we have $\Phi_3 = \pm Re\{(p_1 + i\omega_1 x_1)(p_2 - 2i\omega_1 x_2)^{1/2}\}$.

8. Consider the function $F(P_i, \lambda) = -k\sum_{i=1}^N P_i \ln P_i + \lambda(\sum_{i=1}^N P_i - 1)$, with λ a Lagrange multiplier. The conditional maximum is given by the equations $\partial_{P_i}F = 0, \partial_\lambda F = 0$, which give $P_i = e^{\lambda/k-1}$, the same for all $i = \overline{1, N}$. The maximum is therefore given by the uniform distribution, $P_i = 1/N$.

9. a) The entropy of a system made of two non-interacting subsystems is the sum of entropies: $P_{AB} = P_A P_B \Rightarrow \sum P_{AB}\ln P_{AB} = \sum P_A P_B(\ln P_A + \ln P_B) = (\sum P_A \ln P_A)\sum P_B + (\sum P_B \ln P_B)\sum P_A = \sum P_A \ln P_A + \sum P_B \ln P_B$. Therefore, for our system, $S = Ns$, where $s = -k(\ln(1/2) + \ln(1/2))/2 = k\ln 2$ is the entropy for one spin. Thus, $S = kN\ln 2$.

b) More generally, for a two state system with probabilities P_1, P_2, we get $s = -k[P_1 \ln P_1 + (1 - P_1)\ln(1 - P_1)] = -k[H(e^H - e^{-H})/(e^H + e^{-H}) - \ln(2\cosh(H))] = k[\ln 2 + \ln\cosh H - H\tanh(H)]$. H has been chosen positive here.

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c) Since $\frac{d}{dH}\left[\ln\cosh H - H\tanh(H)\right] = -H/\cosh^2(H) < 0$, we conclude that the entropy is maximum for the symetrical case, $H = 0$ (complete disorder) and minimimum at $H \to \infty$, for a completely ordered system.

10. Use the representation $\delta^N(\mathbf{x}) = \frac{1}{(2\pi)^N}\int d\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{x}}$ and the normalization $\int d\mathbf{k}\, e^{-\alpha(\mathbf{k}-\mathbf{k_0})^2} = (\pi/\alpha)^N$. Then we have $Z \sim [eVh^{-3}N^{-1}(mc)^3]^N E \int d\mathbf{P}\delta(H - E)\delta^N(\mathbf{P} - \mathbf{P_0})$ for large N. Introduce the scalar k_0 and the N vector $\mathbf{k}$ and obtain $Z \sim [eVh^{-3}N^{-1}(mc)^3]^N E_T \int d\mathbf{P} \int d\mathbf{k} \int dk_0 e^{ik_0(\mathbf{P}^2 - 2mE)}e^{i\mathbf{k}\cdot(\mathbf{P}-\mathbf{P_0})}$. Write $k_0\mathbf{P}^2 + \mathbf{k}\cdot\mathbf{P} = k_0[\mathbf{P} + \frac{\mathbf{k}}{2k_0}]^2 - \frac{\mathbf{k}^2}{4k_0}$ and integrate over $\mathbf{P}$. Obtain $Z \sim k_0^{-N/2}\int d\mathbf{k}\int dk_0 e^{-ik_0(2mE)}e^{i\mathbf{k}\cdot(\frac{\mathbf{k}}{4k_0}-\mathbf{P_0})}$. Write $\mathbf{k}^2/4k_0 - \mathbf{k}\cdot\mathbf{P_0} = \frac{1}{4k_0}[\mathbf{k} - 2\mathbf{P_0}k_0]^2 - \mathbf{P_0}^2 k_0$ and integrate over $\mathbf{k}$. Obtain $Z \sim \int dk_0 e^{ik_0(2mE-\mathbf{P_0}^2)}$ and integrate over k_0. Get $Z \sim [eVh^{-3}N^{-1}(mc)^3]^N E_T\delta(2mE - \mathbf{P_0}^2)$. Represent $E_T\delta(2mE - \mathbf{P_0}^2) \sim e^{-N|2mE-\mathbf{P_0}^2|/E}$ and conclude that $S/N \sim kve(mc/h)^3(2mE - \mathbf{P_0}^2)/E$, where $v = V/N$. Conclude that the conjugate force is proportional to the center of mass speed of the system.

11. Use the formula $\frac{\partial}{\partial t}\delta(\vec{x}-\vec{r}(t)) = -\frac{d\vec{r}(t)}{dt}\cdot\nabla\delta(\vec{x}-\vec{r}(t)) = \frac{\vec{p}}{m}\cdot\nabla\delta(\vec{x}-\vec{r}(t))$ to obtain the following local conservation laws:

$$\frac{\partial n}{\partial t} + \nabla\cdot\vec{J}_n(\vec{x},t) = 0 \tag{14}$$

$$\frac{\partial \vec{g}}{\partial t} + \nabla\cdot\vec{J}_g(\vec{x},t) = 0 \tag{15}$$

$$\frac{\partial \epsilon}{\partial t} + \nabla\cdot\vec{J}_e(\vec{x},t) = 0, \tag{16}$$

where the number of particles, momentum and energy density currents are respectively

$$\vec{J}_n(\vec{x},t) = \sum_i \frac{\vec{P}_i}{m}\delta(\vec{x} - \vec{r}_i(t)) \tag{17}$$

$$\vec{J}_g^{\alpha,\beta}(\vec{x},t) = \sum_i \vec{P}_i^{\alpha}\frac{\vec{P}_i^{\beta}}{m}\delta(\vec{x} - \vec{r}_i(t)) \tag{18}$$

$$\vec{J}_e(\vec{x},t) = \sum_i \frac{\vec{P}_i^2}{2m}\frac{\vec{P}_i}{m}\delta(\vec{x} - \vec{r}_i(t)). \tag{19}$$

Note: The momentum density is in fact a symmetric tensor, which gets contracted in equation (2) with the divergence operator.

Now compute the generic average

$$\langle\sum_i f(\vec{P}_i)\delta(\vec{x}-\vec{r}_i(t))\rangle_{\mu c} = \sum_j \frac{\int \prod_i d\vec{p}_i d\vec{q}_i \delta(2mE-\sum_s P_s^2)f(\vec{p}_j)\delta(\vec{x}-\vec{r}_j(t))}{\int \prod_k d\vec{p}_k d\vec{q}_k \delta(2mE-\sum_l P_l^2)} = \frac{N}{V}\langle f(\vec{P}_1)\rangle_{\mu c} \qquad (20)$$

and obtain (see problem 15 in this set for details)

$$\langle n(\vec{x},t)\rangle = \frac{N}{V}, \quad \langle \vec{g}(\vec{x},t)\rangle = \frac{\langle\sum_i \vec{P}_i\rangle}{V} = \vec{0}, \quad \langle \epsilon(\vec{x},t)\rangle = \frac{\langle\sum_i \frac{P_i^2}{2m}\rangle}{V} = \frac{E}{V}, \qquad (21)$$

$$\langle \vec{J}_n(\vec{x},t)\rangle = \vec{0}, \quad \langle \vec{J}_{g,i,j}(\vec{x},t)\rangle = \frac{N\langle P_i P_j\rangle}{V} = \vec{0}, \quad \langle \vec{J}_e(\vec{x},t)\rangle = \frac{\langle\sum_i \frac{P_i^2 \vec{P}_i}{2m}\rangle}{V} = \vec{0}. \qquad (22)$$

Therefore, the identities are identically satisfied, all terms being null.

12. We start by requiring that the constrained function $C(E,N,V,\vec{P}_0,\vec{L}_0) = -kP_i \ln P_i + k\beta(\sum P_i E_i - E) - k\beta p(\sum P_i V_i - V) - k\beta\mu(\sum P_i N_i - N) - k\beta\vec{v}\cdot(\sum P_i\vec{P}_i - \vec{P}_0) - k\beta\vec{\omega}(\sum P_i\vec{L}_i - \vec{L}_0)$ reach a maximum at equilibrium, with the Lagrange multipliers all independent.

The equation $\partial_{P_i}C = 0$ leads to the simple solution

$$P_i \sim e^{-\beta[E_i - pV_i - \mu N_i - \vec{v}\vec{P}_i - \vec{\omega}_i\vec{L}_i]} \qquad (23)$$

and we denote the normalization factor $\sum_i P_i = Z(N,E,V,\vec{P}_0,\vec{L}_0) = e^{-\beta F}$. From $S = -k\sum_i P_i \ln P_i$, we obtain

$$S = k\beta(E - pV - \mu N - \vec{v}\vec{P}_0 - \vec{\omega}\vec{L}_0 + F) \qquad (24)$$

We therefore conclude that $F \sim C$ and it reaches a minimum at equilibrium. This implies that $k\beta = \frac{\partial S}{\partial E} = \frac{1}{T}$, $p = \frac{\partial E}{\partial V}$ (pressure), $\mu = \frac{\partial E}{\partial N}$ (chemical potential), $\vec{v} = \frac{\partial E}{\partial \vec{P}_0}$ (center of mass speed), $\vec{\omega} = \frac{\partial E}{\partial \vec{L}_0}$ (total angular velocity).

13. From the previous problem and the fact that the potential F has an extremum at equilibrium, we get the result

$$C_V = \left(T\frac{\partial S}{\partial T}\right)_V = \left(\frac{E}{T} - \frac{I\vec{\omega}^2}{2T}\right) = Nk\left(\frac{3}{2} - \frac{m\omega^2 R^2}{4kT}\right), \qquad (25)$$

with m the molecular mass and I the moment of inertia of the uniformly distributed gas.

14. a) Following the procedure in 12, we write the partition function

$$Z(N,E,\vec{M}_T) = \left(\int d\vec{m}\, e^{-\frac{\beta\alpha_0}{2}\vec{m}^2 + \beta\vec{h}\vec{m}}\right)^N \qquad (26)$$

Using $\frac{\beta\alpha_0}{2}\vec{m}^2 - \beta\vec{h}\vec{m} = \frac{\beta\alpha_0}{2}[\vec{m} - \frac{\vec{h}}{\alpha_0}]^2 - \frac{\beta\vec{h}^2}{2\alpha_0}$, and $\int d\vec{x}e^{-a\vec{x}^2} = (\frac{\pi}{a})^{3/2}$, we obtain

$$Z(N, E, \vec{M}_T) = \left(\frac{2\pi}{\beta\alpha_0}\right)^{3N/2} e^{\frac{N\beta\vec{h}^2}{2\alpha_0}}. \tag{27}$$

The total magnetization is $\vec{M} = \frac{\partial \ln Z}{\partial \beta\vec{h}} = N\vec{h}/\alpha_0$. For $\vec{h} \sim \vec{0}$, the magnetization is almost null (the system is at maximum disorder), and for $h \to \infty$, almost all spins are aligned with the exterior field (maximum order).

b) $S = k \ln Z + E/T = Nk(\beta\vec{h}^2 - 3/2\ln\beta) +$ constants.

15. Define the generating function

$$F(\vec{k}) = \int \prod_i d\vec{p}_i d\vec{q}_i \delta(2mE - \sum_i p_i^2) e^{i\vec{k}\sum_i \vec{p}_i}, \tag{28}$$

we get

$$\langle \sum_i \vec{p}_i \rangle = \frac{\partial F(\vec{k}=0)}{\partial i\vec{k}}, \quad \langle (\sum_i \vec{p}_i)^2 \rangle = \frac{\partial^2 F(\vec{k}=0)}{\partial(i\vec{k})^2} \tag{29}$$

Writing $\delta(2mE - \sum_i \vec{p}_i^2) = \int dk_0 e^{ik_0(2mE - \sum_i \vec{p}_i^2)}$, and grouping together $-k_0 p_i^2 + \vec{k}\vec{p}_i = -k_0[\vec{p}_i - \frac{\vec{k}}{2k_0}]^2 + \frac{k^2}{4k_0}$, it is easy to see that $\partial_{\vec{k}} \ln F(\vec{k}=0) \sim \vec{k} = \vec{0}$. By exactly the same procedure, one can prove in general that $\langle p_i p_j \rangle = 0, \forall i \neq j$.

Therefore,

$$\langle \sum \vec{p}_i = \vec{0} \rangle, \quad \langle (\sum_i \vec{p}_i)^2 \rangle = \langle \sum_i (\vec{p}_i)^2 + \sum_{i,\alpha \neq j,\beta} \vec{p}_{i\alpha}\vec{p}_{j\beta} \rangle = 2mE. \tag{30}$$

16. From conservation of total energy, $T = (\sum_i N_i T_i)/(\sum_i N_i)$.

17. First compute the partition function for the canonical ensemble,

$$Z_c(N, E, h) = \sum_{all\sigma} e^{\beta h \sum_\sigma} = 2^N \langle e^{2\beta h X - \beta h N} \rangle_{binomial,N,1/2} = 2^N e^{-\beta h N}(e^{2\beta h} + 1)^N = [2cosh(\beta h)]^N \tag{31}$$

where X is a random variable $X = N_u$ giving the total number of spins up, which is obviously distributed binomially, with probability $1/2$ and N states. The expression $\langle e^{tX} \rangle_{binomial}$ can be found in any statistics book.

We obtain for the expectation value of the energy in the canonical ensemble $\overline{E}_c = -\partial_\beta \ln Z_c = Nh\,tanh(\beta h)$. Also, the entropy in the canonical ensemble is $S = k \ln Z + E/T = Nk[\ln 2 + \ln cosh(\beta h) + h\beta\,tanh(\beta h)]$.

Equating the average energy in the two ensembles gives us $\epsilon = tanh(\beta h)$, so temperature can be introduced in the microcanonical ensemble as $\beta h = tanh^{-1}(\epsilon)$, taken as a fixed parameter.

An expansion at small ϵ (high temperature, small external fields) gives for both ensembles $S = Nk[\ln 2 - \epsilon^2]$, showing that the entropy is largest at $T \to \infty$, $\beta = 0$.

18. a) Since the free energy is proportional to the logarithm of the partition function, all constants will be ignored in computing it. We have

$$Z = \left[\int d\vec{r} e^{-\beta r^b} \int d\vec{p} e^{-\frac{\beta p^2}{2m}} \right]^N \sim \left[\int_0^\infty dr r^2 e^{-\beta r^b} \int_0^\infty dr r^2 e^{-\frac{\beta p^2}{2m}} \right]^N. \tag{32}$$

Use the obvious result (obtained through a change of variable) $\int dx x^2 e^{ax^n} \sim a^{\frac{3}{n}}$ and conclude that $Z \sim \beta^{-N\left(\frac{3}{b}+\frac{3}{2}\right)}$. Therefore,

$$E = -\frac{\partial \ln Z}{\partial \beta} = \frac{3NkT}{2}\left(1 + \frac{2}{b}\right) = CT. \tag{33}$$

b) We derive a general result, valid for any conservative external potential $U(\vec{r})$, which can be used in problem 19 as well. The thermal equation of state $pV = NkT$ leads to the local law $p = \frac{\rho}{m}kT$. The mechanical equation of state is simply a statement of equilibrium at each point (see problem 19 for details):

$$dp = -\frac{\rho}{m}\vec{\nabla}U \cdot d\vec{r}. \tag{34}$$

Together, these two equations lead to

$$dp = -\frac{p}{kT}\vec{\nabla}U \cdot d\vec{r} \Rightarrow \ln\frac{p}{p_0} = -\frac{U(\vec{r}) + U(\vec{r}_0)}{kT} \Rightarrow p = p_0 e^{-\frac{U(\vec{r})}{kT}}, \quad n = n_0 e^{-\frac{U(\vec{r})}{kT}}. \tag{35}$$

The normalization factor can be found from the total number of particles,

$$\int d\vec{r} n = N \Rightarrow L^2 \int_0^L dz n_0 e^{-\frac{mgz}{kT}} = N \Rightarrow n_0 = \frac{Ng}{L^2 kT}\frac{1}{1 - e^{-\frac{mgL}{kT}}}. \tag{36}$$

To compute C_v, use the observations noted in part a) and write $Z \sim \left(\int e^{-\frac{\beta p^2}{2m}} d\vec{p} \right)^N \left(e^{-\beta mgz} dz \right)^N \sim \beta^{-\frac{5N}{2}} \Rightarrow C_v = \frac{5Nk}{2}$.

19. The equilibrium average of the momentum density conservation law reads

$$\langle \frac{\partial g_j}{\partial t} \rangle = -\langle \partial^i T_{ij} \rangle + \langle f_j \rangle, \tag{37}$$

where f_j is the local external force density, and T_{ij} is the stress-energy tensor. Stationarity implies setting the time derivative to zero, thus obtaining the local equilibrium law

$$\langle \partial^i T_{ij} \rangle = \langle f_j \rangle. \tag{38}$$

Integarting this equation for diagonal stress-energy tensors $T_{ij} = p\delta_{ij}$, we obtain

$$\langle dp \rangle = \langle f_j dx^j \rangle. \tag{39}$$

The force density is given by $-\frac{\rho}{m}\vec{\nabla}U$, so the results of problem 18 apply.

20. As shown in homework set 3, the probability distribution function is $P \sim e^{-\beta(\sum_i p_i^2/2m - \vec{v}\cdot\sum_i \vec{p_i})}$, where $\vec{v} = \frac{\vec{P_0}}{Nm}$ is the center of mass speed. The probability distribution function is the product of N identical functions, so we have

$$\langle \sum_i \vec{v_i}\frac{mv_i^2}{2} \rangle = \frac{N}{2m^2}\langle \vec{p}^2\vec{p} \rangle, \tag{40}$$

computed with the probability distribution function $P \sim e^{-\beta(p^2/2m - vp_z)}$, where we have chosen the z direction parallel to the direction of $\vec{v}$.

Noting that

$$\int e^{-\beta\frac{p_x^2}{2m}} p_x^{2n+1} dp_x = 0 \tag{41}$$

for any positive integer n, we obtain $\langle p^2 p_{x,y} \rangle = 0$. As for the remaining component, we will use the following formulae:

$$\int e^{-\beta\frac{p_z^2}{2m}+\beta vp_z} p_z^n dp_z = \frac{\partial^n}{\beta^n \partial v^n} \int e^{-\beta\frac{p_z^2}{2m}+\beta vp_z} dp_z, \quad \int e^{-\beta\frac{p_z^2}{2m}+\beta vp_z} dp_z = \sqrt{\frac{2\pi m}{\beta}} e^{\frac{\beta mv^2}{2}} \tag{42}$$

We obtain

$$\int e^{-\beta\frac{p_z^2}{2m}+\beta vp_z} dp_z = \sqrt{\frac{2\pi m}{\beta}}, \quad \int e^{-\beta\frac{p_z^2}{2m}+\beta vp_z} p_z dp_z = \sqrt{\frac{2\pi m}{\beta}} mv, \int e^{-\beta\frac{p_z^2}{2m}+\beta vp_z} p_z^2 dp_z = \sqrt{\frac{2\pi m}{\beta}}\left(\frac{m}{\beta}+m^2v^2\right), \tag{43}$$

$$\int e^{-\beta\frac{p_z^2}{2m}+\beta vp_z} p_z^3 dp_z = \sqrt{\frac{2\pi m}{\beta}}\left(\frac{3m^2v}{\beta}+m^3v^3\right). \tag{44}$$

Therefore,

$$\langle p_{x,y}^2 p_z \rangle = \frac{m^2v}{\beta}, \quad \langle p_z^3 \rangle = \frac{3m^2v}{\beta}+m^3v^3, \quad \langle J_E^z \rangle = \frac{N}{2m^2}\left(\frac{5m^2v}{\beta}+m^3v^3\right) = \frac{5NkTv}{2}\left(1+\frac{mv^2}{5kT}\right). \tag{45}$$

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21. Let $f(\{\vec{r_i}\})$ be any differentiable function of the coordinates of the system of particles, then applying the operator U leads to

$$U_{P_T^z}(z_0)f = \sum_{k=0}^{\infty} \frac{z_0^k}{k!} \left(\sum_{i=1}^{N} \frac{\partial}{\partial \vec{r_i}^z} \right)^k f = f(\{\vec{r_i} + z_0\hat{z}\}), \tag{46}$$

from the usual form of the Taylor expansion of functions of multiple variables. The operator U is a finite translation operator along the z axis.

22. Rewrite Hooke's Law in matrix notation as

$$-\sigma = \left(B - \frac{2\mu}{3} \right) Trace U Id + 2\mu U \tag{47}$$

and assume infinitesimal displacements $-dz, da$ along the z and x, y, respectively. The law becomes

$$-\sigma_z = \left(B - \frac{2\mu}{3} \right)(-dz/L + 2da/a) - 2\mu dz/L, \quad -\sigma_{x,y} = \left(B - \frac{2\mu}{3} \right)(-dz/L + 2da/a) + 2\mu da/a. \tag{48}$$

Now write the energy due to external pressure as

$$dE = pdV = p(-a^2 dz + 2aLda) = -pV_0 \frac{dz}{L} + 2pV_0 \frac{da}{a} \tag{49}$$

Therefore, $\sigma_z = -\frac{\partial E}{\partial dz/L} = -\sigma_{x,y} = pV_0$. Solving the system of equations

$$-pV_0 = \left(B - \frac{2\mu}{3} \right)(-dz/L + 2da/a) - 2\mu dz/L = \left(-B + \frac{2\mu}{3} \right)(-dz/L + 2da/a) - 2\mu da/a, \tag{50}$$

we obtain $dz = pL^2 a^2 (2B - \mu/3)/(3B\mu), \quad da = pLa^3 (B + \mu/3)/(3B\mu)$

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23. The Gibbs-Duhem relation gives

$$Ed\frac{1}{T} + Vd\frac{p}{T} - Nd\frac{\mu}{T} = 0, \tag{51}$$

from which we find by applying the equations of state

$$d\frac{\mu}{T} = \frac{E}{N}d\frac{1}{T} + \frac{V}{N}d\frac{p}{T} = \frac{3k}{2}d\ln\frac{N}{E} + kd\ln\frac{N}{V} = kd\ln\left[\left(\frac{N}{E} \right)^{3/2} \frac{N}{V} \right] \tag{52}$$

We conclude that the new equation of state is $(Ne = E, Nv = V)$:

$$\frac{\mu}{T} = k \ln \left[\frac{(e)^{3/2} v}{\hbar} \right], \tag{53}$$

where the Planck constant has been introduced for dimensional purposes and purely numerical integration constants have been ignored. We also obtain

$$S = \frac{5Nk}{2} + Nk \ln \left[\frac{(e)^{3/2} v}{\hbar} \right]. \tag{54}$$

24. a) Since S is null at $T = 0$ regardless of the other variables, it has an expansion in positive powers of the temperature,

$$S(T, \ldots) = \sum_{k_i > 0, i \in Z_+} T^{k_i} f_i(\ldots), \tag{55}$$

where $\ldots$ signify the other arguments of S. The heat capacity then has the expansion

$$C(T) = T \frac{\partial S}{\partial T} = \sum_{k_i > 0, i \in Z_+} T^{k_i} k_i f_i(\ldots) \tag{56}$$

and vanishes at $T = 0$.

b) From the Maxwell relation

$$\left(\frac{\partial V}{\partial T} \right)_p = - \left(\frac{\partial S}{\partial p} \right)_T, \tag{57}$$

and the expansion in (5), we obtain

$$\alpha \sim \sum_{k_i > 0, i \in Z_+} T^{k_i} \left(\frac{\partial f_i}{\partial p} \right)_T \tag{58}$$

which evidently vanishes at 0 as well.

25. Using the equations of state for the ideal gas, we have

$$dS = \frac{3Nk}{2T} dT + \frac{Nk}{V} dV \Rightarrow T \left(\frac{\partial S}{\partial T} \right)_p = \frac{3Nk}{2} + Nk \left(\frac{\partial \ln V}{\partial \ln T} \right)_p, \quad T\alpha = \left(\frac{\partial \ln V}{\partial \ln T} \right)_p, \quad p\kappa_T = - \left(\frac{\partial \ln V}{\partial \ln p} \right)_T \tag{59}$$

Using again the equation of state in the form $\ln V = \ln T - \ln p + \ln(Nk)$, we obtain $C_p = 5Nk/2$, $\alpha = 1/T$, $\kappa_T = 1/p$.

26. Since N is kept constant in all the derivatives, we drop the symbol. Using the jacobian notation, we have

$$cc^2 = -\frac{V^2}{mN}\left(\frac{\partial p}{\partial V}\right)_S = -\frac{V^2}{mN}\frac{(p,S)}{(V,S)} \tag{60}$$

$$C_p = T\frac{(S,p)}{(T,p)} \tag{61}$$

$$C_v = T\frac{(S,V)}{(T,V)} \tag{62}$$

$$\alpha V = \frac{(V,p)}{(T,p)} \tag{63}$$

$$\kappa_T V = -\frac{(V,T)}{(p,T)} \tag{64}$$

Now write

$$\frac{(p,S)}{(V,S)} = \frac{(p,S)}{(p,T)}\cdot\frac{(p,T)}{(V,T)}\cdot\frac{(V,T)}{(V,S)} = -\frac{C_p}{T}\frac{1}{\kappa_T V}\frac{T}{C_v} \Rightarrow c^2 = \frac{V}{mN\kappa_T}\frac{C_p}{C_v} = \frac{\gamma}{\kappa_T\rho}, \tag{65}$$

where $\rho = mN/V$ is the fluid density, $\gamma = C_p/C_v$ is the adiabatic coefficient of the fluid, and $B = 1/\kappa_T$ is its elasticity modulus. As the book shows, there is a Mayer identity, $C_p = C_v + \frac{TV\alpha^2}{\kappa_T}$.

27. Since V is kept constant in all the functions of interest, we ignore the differential pdV throughout the computations. From

$$dE = TdS - hdM, \tag{66}$$

we obtain

$$T\left(\frac{\partial S}{\partial E}\right)_M = 1, \quad T\left(\frac{\partial S}{\partial E}\right)_h = 1 + h\left(\frac{\partial M}{\partial E}\right)_h \tag{67}$$

We also have

$$\left(\frac{\partial M}{\partial E}\right)_h = \left(\frac{\partial M}{\partial T}\right)_h\left(\frac{\partial T}{\partial E}\right)_h = \frac{\kappa_T V}{C_v} \tag{68}$$

We obtain

$$\left(\frac{\partial S}{\partial E}\right)_h = \left(\frac{\partial S}{\partial E}\right)_M\left(1 + \frac{h\kappa_T V}{C_v}\right) \tag{69}$$

Since (use jacobians)

$$\left(\frac{\partial S}{\partial E}\right)_h \Big/ \left(\frac{\partial S}{\partial E}\right)_M = \left(\frac{\partial h}{\partial M}\right)_S \Big/ \left(\frac{\partial h}{\partial M}\right)_E = \frac{\chi}{\chi_S}, \tag{70}$$

we conclude that

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$$\chi = \chi_S \left(1 + \frac{h\kappa_T V}{C_v}\right) \tag{71}$$

28. Since system B is at fixed temperature, its thermodynamical potential is the entropy itself, so S_B is maximized and E_B is fixed. From

$$T(S_A + S_B) - E_A + E_B = const. \tag{72}$$

we conclude that, at fixed generalized forces, S_B will reach a maximum and $E_A - TS_A$ a minimum. In the information-theoretic approach, the function to be maximized is obtained from the entropy and the constraints on the average thermodynamic forces $\overline{F^j}$, introduced through Lagrange multipliers μ_j:

$$W = \sum_i P_i \ln P_i - \sum_j \frac{\mu_j}{T} \sum_i P_i F_i^j \tag{73}$$

should reach a maximum. Therefore, $-WT = \Gamma(\overline{F^j}) = -TS + \sum_j \mu_j \overline{F^j}$ is the appropriate thermodynamic potential.

29. Assume the volume becomes $V = V_0 + LA$ and that the external pressure is null. Since there is no heat exchange, the variation of the energy is given by

$$\Delta E = -\frac{kL^2}{2} = \frac{3Nk}{2}[T_0 - T] = \frac{3p_0 V_0}{2T_0}[T_0 - T] \Rightarrow T = T_0 \left[1 - \frac{kL^2}{3p_0 V_0}\right]. \tag{74}$$

The Clapeyron-Mendeleev equation of states gives

$$\frac{p_0 V_0}{T_0} = \frac{kL(V_0 + AL)}{AT} \Rightarrow p_0 V_0 \left[1 - \frac{kL^2}{3p_0 V_0}\right] = \frac{kL(V_0 + AL)}{A} \tag{75}$$

Solving the quadratic equation in L, one gets

$$\frac{kL}{3Ap_0} = \frac{-\frac{kV_0}{A} + \sqrt{(\frac{kV_0}{A})^2 + \frac{16kp_0 V_0}{3}}}{8Ap_0}, \quad \frac{kL^2}{3p_0 V_0} = \frac{1}{4}\left(1 - \frac{kL}{Ap_0}\right) \tag{76}$$

In conclusion,

$$T = \frac{3T_0}{4}\left[1 - \frac{-\frac{kV_0}{A} + \sqrt{(\frac{kV_0}{A})^2 + \frac{16kp_0 V_0}{3}}}{8Ap_0}\right] \tag{77}$$

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30. From $TS = E - F$ and $E_1 + E_2 = E_{final}$, we conclude

$$-S_{final} + S_1 + S_2 = (\beta F)_{final} - \beta_1 F_1 - \beta_2 F_2 \tag{78}$$

where $(N_1 + N_2)/\beta = N_1/\beta_1 + N_2/\beta_2$. We also have $\beta F = N \ln(\beta^{3/2} n)+$ constants, where n is the particle concentration. Therefore, for the initial state we have (up to constants that do not change the variation of entropy):

$$\beta_1 F_1 + \beta_2 F_2 = N_1 \ln(n_1 \beta_1^{3/2}) + N_2 \ln(n_2 \beta_2^{3/2}) \tag{79}$$

Case 1: Identical species.

In this case, we compute the variation of entropy by the formula:

$$-\Delta S = N \ln(n\beta^{3/2}) - \sum_{i=1,2} N_i \ln(n_i \beta_i^{3/2}), \tag{80}$$

where $n = (n_1 + n_2)/2$ and $T(N_1 + N_2) = T_1 N_1 + T_2 N_2$. The sign of ΔS is obtained by comparing the argument of the logarithm to 1, i.e. computing the ratio

$$\left\{ \frac{[(N_1 + N_2)T_1]^{N_1}[(N_1 + N_2)T_2]^{N_2}}{[N_1 T_1 + N_2 T_2]^{N_1+N_2}} \right\}^{3/2} \frac{(N_1 + N_2)^{N_1+N_2}}{2^{N_1+N_2} N_1^{N_1} N_2^{N_2}} \tag{81}$$

For the special case $T_1 = T_2 = T$, $N_1 = N_2 = N/2$, we obtain $\Delta S = 0$.

Case 2: Distinguishable species.

The formula now reads

$$-\Delta S = \left\{ \frac{(N_1 T_1 + N_2 T_2)^{N_1+N_2}}{(N_1 + N_2)^{N_1+N_2} T_1^{N_1} T_2^{N_2}} \right\}^{3/2} - (N_1 + N_2) \ln 2 \tag{82}$$

One can prove that $\Delta S > 0$ along the following line of reasoning: first, prove that for given $N_{1,2}$, the variation is minimal at $T_1 = T_2 = T$ by simply taking the derivatives in T_1, T_2 (remember that $T = T(T_1, T_2)$) and showing that the extremum is obtained at $T_1 = T_2$:

$$\partial_{T_1} \Delta S = \frac{3}{2} \left(N_1 \frac{N_1 + N_2}{N_1 T_1 + N_2 T_2} - N_1 \frac{N_1}{T_1} \right) \tag{83}$$

Clearly, the derivative vanishes iff. $T_1 = T_2$. Computing the determinant of the second order derivatives matrix is a straightforward way of showing that the extremum is indeed a maximum. By exactly the same method, one can prove that in case 1, $\Delta S \geq 0$, with no change in entropy at $T_1 = T_2 = T$.

In case 2, at $T_1 = T_2$, one gets $\Delta S = (N_1 + N_2) \ln 2 > 0$.

31. In each compartment, the reaction equilibrium imposes

$$\frac{n_A n_B}{n_c} = \left(\sqrt{\frac{m_A m_B}{\hbar^2 2\pi\beta m_C}}\right)^3 =_{def} \frac{1}{V_0} \tag{84}$$

Equilibrium of partial pressure for species A, C imposes $n_A^{(1)} = n_A^{(2)}$, $n_C^{(1)} = n_C^{(2)}$, so we obtain the result that concentrations of particles are the same in the two compartments. Next, use $n_A = n_B$ due to symmetry of the reaction and $n_A + n_B + n_C = n_0$, where n_0 is the initial concentration of particles in each compartment. We obtain a quadtratic equation in n_A:

$$V_0 n_A^2 + 2n_A - n_0 = 0, \tag{85}$$

which has only one positive solution. Then find n_C from $2n_A + n_C = n_0$.

32. Because the temperatures are equal and the total energy is conserved, we obtain as in problem 28,

$$\Delta S = \beta(F_i - F_f), \tag{86}$$

and

$$\beta F_i = N_1 \ln n_1 + N_2 \ln n_2 + const. \tag{87}$$

Case 1: different masses.
We have

$$\beta F_f = N_1 \ln f_1 n_1 + N_2 \ln f_2 n_2, \tag{88}$$

where $f_{1,2} = V_{1,2}/(V_1 + V_2)$, and $V_{1,2}$ are the volumes occupied initially by the two gases. Clearly, $f_{1,2} < 1$ and

$$\Delta S = N_1 \ln(1/f_1) + N_2 \ln(1/f_2) > 0. \tag{89}$$

Case 2: identical molecules.
We get

$$\beta F_f = (N_1 + N_2) \ln(n_1 f_1 + n_2 f_2) \tag{90}$$

Equal densities $n_1 = n_2 = n$ leads to $\beta F_f = (N_1 + N_2) \ln[n(f_1 + f_2)] = N \ln n$, $\beta F_i = (N_1 + N_2) \ln n = N \ln n$, so $\Delta S = 0$. Since the temperature, density and therefore pressure are identical in the two compartments, the partition is equivalent to a virtual partition, which does not change the total number of configurations for the whole system, so the entropy does not change under removal (or any fluctuation) of the partition.

33. Adding the coupling term $-h\psi$ to the free energy allows to find the inverse susceptibility in the limit $h \to 0$, $T \to T_c$:

$$h = (a_2 + a_4\psi^2 + a_6\psi^4)\psi \Rightarrow \chi^{-1} = a_2 + 3a_4\psi^2 + 5a_6\psi^4. \tag{91}$$

Case 1: $T > T_c$. All the terms in the free energy are positive, so the minimum is achieved for $\psi = 0$. We also obtain $\chi = \frac{1}{a_2^0(T-T_c)}$.

Case 2: $T < T_c$. Minimizing the free energy leads to the equation

$$\psi(a_6\psi^4 + a_4\psi^2 - |a_2|) = 0. \tag{92}$$

There are two solutions close to the origin, $\psi_1 = 0$ and $\psi_2 = \pm\sqrt{\frac{|a_2|}{a_4}}$. Since

$$\frac{F}{V}(\psi_2) - \frac{F}{V}(\psi_1) = \psi_2^2(-\frac{|a_2|}{2} + \frac{|a_2|}{24} + O(\psi^4)) < 0, \tag{93}$$

we conclude that ψ_2 actually minimizes the free energy. Notice that there are two degenerate solutions, corresponding to the two possible orientations of the average magnetization (classical degeneracy). For the susceptibility we have

$$\chi = \frac{1}{a_2 + 3|a_2|} = \frac{1}{2a_2^0|T - T_c|}. \tag{94}$$

34. Write

$$\frac{F}{V} = -|r|f^2 + \frac{u}{2}f^4 - \frac{\nu f^p}{p}\cos(ps) \tag{95}$$

and find the configuration of minimum from the equations $\partial_f F = 0 = \partial_s F$. From these equations we obtain $\sin(ps) = 0 \Rightarrow s_k = \frac{k\pi}{p}, k = 0, \ldots, 2p - 1$ and

$$f\left(-2|r| + 2uf^2 - \nu(-1)^k f^{p-2}\right) = 0 \tag{96}$$

If $p = 4$, we have $(f^2)_{1,2} = \frac{2|r|}{2u\pm|\nu|}$, depending on the sign of the term $(-1)^k$. The value of the free energy for these two solutions is

$$\frac{F_{1,2}}{V} = -|r|\psi^2\left(1 - \frac{2u \pm |\nu|}{2(2u \pm |\nu|)}\right) = -\frac{r^2}{2u \pm |\nu|} \tag{97}$$

Clearly, if the solution corresponding to $+|\nu|$ is chosen, then the free energy is negative and we obtain ordering for any ν. For the other set of solutions, we must impose the constraint $|\nu| < 2u$.

In this set, χ is the magnetic susceptibility per particle, where appropriate.

35. Case 1: One dimensional Ising model.

In this case there is no phase transition at finite temperatures, so all the thermodynamical quantities should be free of discontinuities. Replacing the spin variable with the average magnetization m leads to the following partition function:

$$Z_N = \left[\sum_{\{\sigma\}} e^{\beta(Jm+B)\sigma} \right]^N, \tag{98}$$

so that $\log Z_N = N \log \cosh[\beta(Jm + B)]+$ constants. The mean field equation reads

$$Nm = \frac{1}{\beta} \frac{\partial \log Z_N}{\partial B} \Rightarrow m = \tanh[\beta(Jm + B)]. \tag{99}$$

At $B = 0, T \to 0$ we choose the solution $m = 0$ because it is the right solution for large T and the free energy is an analytic function, which cannot lead to a phase transition (spontaneous magnetization). Moreover, $\chi = \frac{\partial m}{\partial B}|_{B=0} = \frac{\beta}{\cosh^2(\beta Jm)}$.

Case 2: Ising model in higher dimensions.

In the following we develop the mean field theory for the Ising model in dimensions 2 and higher. The question is thoroughly treated in the textbook, so we present a slightly different approach, leading to the same set of critical exponents. The point is that, regardless of the approximation used in deriving the mean field results, the critical exponents should be the same. Therefore, we can use the formal result derived in part 1, where $J = k_B T_c$ is now understood as incorporating the sum over nearest neighbors. Even though the partition function is *not* the same as obtained by the standard saddle point equation, we should still obtain the same critical exponents.

The equation

$$m = \tanh \left[\frac{T_c}{T} m + \beta B \right] \tag{100}$$

can be solved in the neighborhood of $T = T_c, B = 0, m = 0$ by the expansion

$$\tanh x \simeq x - \frac{x^3}{3} + O(x^5), \tag{101}$$

leading to the equation

$$m = \left[\frac{T_c}{T} m + \beta B \right] - \frac{\left[\frac{T_c}{T} m + \beta B \right]^3}{3}. \tag{102}$$

To find the zero-field magnetization set $B = 0$ and obtain

$$m\left[\frac{T - T_c}{T} + \frac{m^2 T_c^3}{3T^2}\right] = 0. \tag{103}$$

Clearly, for $T > T_c$, the only real solution is $m = 0$. For $T < T_c$, we also have the non-zero solutions

$$m = \pm\sqrt{\frac{3T^2|T - T_c|}{T_c^3}}, \tag{104}$$

which minimize the energy. We therefore obtain in the ferromagnetic phase $m_{MF} \sim |T - T_c|^{1/2}$, as expected.

Computation of the magnetic susceptibility is similar: taking a derivative with respect to the external field in (5) leads to the equation

$$\chi = \left(\frac{T_c}{T}\chi + \frac{1}{k_B T}\right)\left[1 - \left(\frac{T_c}{T}m + \beta B\right)^2\right] \tag{105}$$

Above T_c, we have the solution $m(B = 0) = 0$ so the equation becomes

$$\chi\left(1 - \frac{T_c}{T}\right) = \beta \Rightarrow \chi = \frac{1}{k_B|T - T_c|}. \tag{106}$$

For $T < T_c$, substitution of the solution $m^2 = \frac{3T^2(T_c - T)}{T_c^3}$ gives

$$\chi\left[1 - \frac{T_c}{T} + 3\frac{T_c - T}{T}\right] = \beta\left[1 - \frac{3(T_c - T)}{T_c}\right] \tag{107}$$

We therefore obtain for the leading singularity

$$\chi = \frac{1}{2k_B|T - T_c|}. \tag{108}$$

As expected, the universal values of the critical exponents in the mean field approximation are obtained.

36. Case 1: Heisenberg system at $T \to 0$.

At zero external field and low temperatures, the Heisenberg system has a ground state where all spins are aligned (say, along the z axis). Therefore, the ground state energy is simply $E = -NJ\sum_{<>}$ and depends on the type of lattice considered. Perturbations about this ground state amount to slight deviations of the individual spins from the z directions, and they are described by the following (cosine expanded) dispersion relation

$$\epsilon_k = 2Ja^2 k^2, \tag{109}$$

where a is the lattice constant and k is the wave number for the perturbation of energy ϵ_k. Therefore, the perturbations about the ground state can be described by Bose statistics (see textbook, $s = 2$), with the dispersion relation indicated above and will lead to the perurbation energy

$$\Delta E \sim \int dk \frac{k^4}{e^{2J a^2 \beta k^2} - 1} \sim \beta^{-5/2}. \tag{110}$$

We therefore obtain the temperature dependence $C_V \sim T^{3/2}$ for the spin waves in three dimensions.

Case 2: Heisenberg system near the critical point. In the mean field approximation, the energy is read directly from the saddle point expression of the partition function:

$$\langle E \rangle = -N\overline{J}m^2. \tag{111}$$

Alternatively, one can use $F_{MF} = -Nk_B T \ln \frac{\sinh(\beta \overline{J} m)}{\beta \overline{J} m}$, $\quad E = F - T\frac{\partial F}{\partial T}$ to get

$$E = -N\overline{J}m L(\beta \overline{J} m) = -N\overline{J}m^2. \tag{112}$$

Since $m = 0$ above T_c, we obtain $E = 0$, $\quad C_V = 0$ above T_c. This should not be surprising, since the system is at maximum disorder above T_c and C_V is porportional to the increase in entropy with temperature.

Below T_c, we have from the general mean field approach $m^2 \sim T^2(T_c - T)$, so that the temperature dependence becomes

$$E = -N\overline{J}k_B \frac{T^2(T_c - T)}{T_c^2}, \quad C_V = Nk_B + O(|T - T_c|). \tag{113}$$

37. Assume a density of states given by $s = 1/2$. We will be using standard results already derived in the textbook. The potential can be derived from the energy of the system, $\Omega = -\frac{2E}{3}$. As the textbook indicates, the low temperature expansion of the energy for fermions and bosons (assume no Bose-Einstein condensation) are respectively

$$E_f = E(0) + \frac{n\pi^2}{4}\left(\frac{\overline{D}}{3n}\right)^{2/3}(k_B T)^2 V, \quad E_b = E(0) - \frac{3n|\mu|}{2}\left(\frac{k\overline{D}}{n}\right)^2 (k_B T)^{3/2} V, \tag{114}$$

where n is the particle density and $k = \Gamma(3/2)\zeta(3/2)$. We obtain for the quantum corrections of the thermodynamical potential

$$\Omega_f = -p_{cl}V - \left[\frac{n\pi^2}{6}\left(\frac{\overline{D}}{3n}\right)^{2/3}(k_B T)^2\right]V, \quad \Omega_b = -p_{cl}V + \left[kn|\mu|\left(\frac{k\overline{D}}{n}\right)^2 (k_B T)^{3/2}\right]V. \tag{115}$$

As can be seen from these formulas, the quantum corrections show that the pressure of the system of fermions is larger than the classical value, while for the system of bosons, it is smaller. This is usually explained as an effect of the additional repulsion induced by the Pauli principle in the case of fermions, and the contrary effect in the case of bosons (counting of states for symmetrical, antisymmetrical, and classical systems).

38. We first find the density of states for 1-D photons: $D(\epsilon)d\epsilon = \frac{dp}{\pi\hbar}V$ (polarization factor included). From the dispersion relation $\epsilon = cp$ we obtain $D(\epsilon) = \frac{L}{\pi\hbar c}$, where L is the 1-D volume occupied by the photons. The energy is then

$$E = \frac{L}{\pi\hbar c}\int d\epsilon\frac{\epsilon}{e^{\beta\epsilon}-1}, \tag{116}$$

which can be computed by using the expansion

$$\frac{1}{e^{\beta\epsilon}-1} = e^{-\beta\epsilon}\sum_{k=0}^{\infty}e^{-k\beta\epsilon} \tag{117}$$

Using also the formula $\int d\epsilon e^{-k\beta\epsilon}\epsilon = \frac{1}{k^2\beta^2}$, we can write

$$E = \frac{L(k_BT)^2}{\pi\hbar c}\sum_{k=1}^{\infty}\frac{1}{k^2} = \frac{\pi Lk_B^2T^2}{12\hbar c} \tag{118}$$

The first term in the expansion for the heat capacity is then $C_V = \frac{\pi Lk_B^2T}{12\hbar c}$.

39. i) The extremum condition satisfied by the free energy reads

$$\partial_\alpha F = 0 \Rightarrow \psi_\alpha[r + u|\psi|^2] = 0. \tag{119}$$

Depending on the sign of $r(T)$, we have the disordered phase $T > T_c$, $\psi_\alpha = 0$, $F = 0$ and the ordered phase, $T < T_c$, $|\psi|^2 = |\frac{r}{u}|$.

ii) To simplify the derivation, note that by the Leibniz rule,

$$\partial_\alpha\partial_\beta g^2 = 2[\partial_\alpha g\partial_\beta g + g\partial_\alpha\partial_\beta g], \tag{120}$$

for any doubly differentiable function g. The we get

$$\partial_\alpha\psi_\beta^2 = 2\delta_{\alpha\beta}\psi_\beta, \quad \partial_\alpha\partial_\beta\psi_\gamma^2 = 2\delta_{\alpha\beta}\delta_{\alpha\gamma}, \quad \partial_\alpha\partial_\beta(|\psi|^2)^2 = 2[\partial_\alpha|\psi|^2\partial_\beta|\psi|^2 + |\psi|^2\partial_\alpha\partial_\beta|\psi|^2] = 4[\delta_{\alpha\beta}|\psi|^2 + 2\psi_\alpha\psi_\beta] \tag{121}$$

Using the above relations, we obtain

$$\chi_{\alpha\beta}^{-1} = [r + u|\psi|^2]\delta_{\alpha\beta} + 2u\psi_\alpha\psi_\beta. \tag{122}$$

Case 1: Disordered Phase.

Since $\psi = \vec{0}$, we get the homogenuous symmetric tensor

$$\chi^{-1} = \begin{bmatrix} r & 0 & 0 \\ 0 & r & 0 \\ 0 & 0 & r \end{bmatrix} \tag{123}$$

Case 2: Ordered Phase.

Substitution of $\psi_\alpha = M\delta_{3,\alpha}$ with the condition $r + uM^2 = 0$ gives the planar circularily symmetric tensor

$$\chi^{-1} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2|r| \end{bmatrix} \tag{124}$$

The interpretation of this result is profound. Above T_c, the system is invariant under the group of orthogonal transformations in 3 dimensions. All the quadratic terms in the free energy have the same coefficients (which can be identified with masses of the modes ψ_α). Below T_c, the system undergoes a spontaneous symmetry breaking process, and is left with the residual planar symmetry of orthogonal transformations in 2 dimensions. The modes corresponding to the reduced symmetry group (also known as the little group of the vector $\psi(T < T_c)$) have zero masses $(\chi_{xx}^{-1}, \chi_{yy}^{-1})$, so fluctuations in the XY plane can be excited with arbitrarily small external fields.

40. Since all derivatives are taken with respect to the temperature only, we will label all quantities which are temperature independent as constants. We have $E = -\frac{\partial \log Z_N}{\partial \beta} = k_B T^2 \frac{\partial \log Z_N}{\partial T}$, and $\log Z_N = N \log Z_1 +$ constants.

To compute Z_1 as a function of temperature, write

$$Z_1 = \prod_{i=1}^r \int dq e^{-\frac{\beta K_i q^2}{2}} \prod_{j=1}^s \left(\int dp e^{-\frac{\beta p^2}{2m_j}} \right)^3 \cdot constants, \tag{125}$$

so that by a simple coordinate transformation we obtain the desired temperature dependence:

$$Z_1 = T^{\frac{3s+r}{2}} \cdot constants. \tag{126}$$

The average energy thus becomes $E = \frac{(3s+r)Nk_B}{2}T^2\frac{\partial \log T}{\partial T} = (3s+r)N\frac{k_B T}{2}$. We also get $C_V = (3s+r)N\frac{k_B}{2}$.

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Physics 352

Spring 2003

Problem Set 8 - Solutions

June 6, 2003

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Note: Graded homework will be available for pick-up today at 1:00 PM, in KPTC 101 (the east side wall).

41. Write the dispersion relation in the form $D(\epsilon) = \overline{D}\epsilon^s$ and derive from $D(\epsilon)d\epsilon \sim pdp$, $\quad d\epsilon \sim pdp$ that $s = 0$, $D(\epsilon) = \overline{D}$.

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a) The thermodynamic potential becomes

$$\Omega = \frac{\overline{D}V}{\beta} \int d\epsilon \ln[1 - e^{-\beta(\epsilon + |\mu|)}], \tag{127}$$

where we have emphasized the fact that $\mu \leq 0$ for bosons. Using the expansion $\ln[1 - t] = -\sum_{n \geq 1} \frac{t^n}{n}$, we get

$$\Omega = -\frac{\overline{D}V}{\beta} \sum_{n \geq 1} \frac{e^{-n\beta|\mu|}}{n} \int d\epsilon e^{-n\beta\epsilon} = -\frac{\overline{D}V}{\beta^2} \sum_{n \geq 1} \frac{e^{-n\beta|\mu|}}{n^2}. \tag{128}$$

b, c) Use $N = -\frac{\partial \Omega}{\partial \mu}$ to get

$$n = \frac{N}{V} = \frac{\overline{D}}{\beta} \sum_{n \geq 1} \frac{e^{-n\beta|\mu|}}{n} = -\frac{\overline{D}}{\beta} \ln[1 - e^{-\beta|\mu|}]. \tag{129}$$

In other words, $1 - e^{-\beta|\mu|} = e^{-\frac{\beta n}{D}}$, and since n must be finite even in the thermodynamic limit, we conclude that $\mu \neq 0$ for all finite values of β.

d) The phase transition can only occur if the number of states available at $p = 0$ is macroscopically large. This is directly related to a finite discontinuity in the density of states at $\epsilon = 0$, which can be represented through the step function and leads to the contribution at $\epsilon = 0$. The discontinuity of the density of states at $\epsilon = 0$ can only come from dimensional considerations; the geometrical meaning of this analysis is related to the problem of filling a $d-$ dimensional sphere (in p space) with a fluid of density p^{d-s}.

42. The dispersion relation can be written in the form $D(\epsilon) \sim p^3 \frac{dp}{d\epsilon} \sim p^2 \sim \epsilon$, so $D(\epsilon) = \overline{D}\epsilon$. Equation (1051) reads

$$N = V\overline{D} \int d\epsilon \frac{\epsilon}{e^{\beta_0 \epsilon} - 1} = Vk\overline{D}(\beta_0^2), \tag{130}$$

and $k = \zeta(2)$. Therefore, $\beta_0 \sim \sqrt{n}$. By dimensional analysis, we can always write (up to numerical constants) $\beta_0 \sim \frac{\hbar^2}{2ml^2}$, where $l^{-2} = \sqrt{n}$.

43. From the average occupancy number $n_{p,\sigma} = \frac{1}{e^{\beta(\epsilon_p - \mu B\sigma)} + 1}$, we derive the magnetization

$$\langle M \rangle \sim \int dp \left[\frac{1}{e^{\beta(\epsilon_p - \mu B)} + 1} - \frac{1}{e^{\beta(\epsilon_p + \mu B)} + 1} \right] = \int dp \frac{2e^{\beta\epsilon_p} \sinh(\beta\mu B)}{1 + 2e^{\beta\epsilon_p} \cosh(\beta\mu B) + e^{2\beta\epsilon_p}} \tag{131}$$

We can write

$$\langle M \rangle \sim \frac{1}{\beta\mu} \int dp \frac{\partial}{\partial B} \ln[1 + 2e^{\beta\epsilon_p} \cosh(\beta\mu B) + e^{2\beta\epsilon_p}] \tag{132}$$

The logarithm can be expanded and leads to an expression of the type

$$\ln[1 + 2e^{\beta\epsilon_p} \cosh(\beta\mu B) + e^{2\beta\epsilon_p}] = 2\beta\epsilon_p + 2e^{-\beta\epsilon_p} \cosh(\beta\mu B) + O(e^{-2\beta\epsilon_p})), \tag{133}$$

so in the zero field limit, we have $\langle M \rangle = \sinh(\beta \mu B)$ and $\chi = \beta \mu \cosh(\beta \mu B)$. At finite β and $B = 0$, we get $\langle M \rangle = 0$, $\chi = \frac{\mu}{k_B T}$. However, if $T \to 0$, we see that any infinitesimal external field orients the spins parallel to it, so at $T = 0, B = 0$, $\langle M \rangle = \pm 1$, depending on how $B = 0$ is approached.

44. i) Conservation of total energy reads

$$\left[\frac{N_1^{5/3}}{V_1^{2/3}} + \frac{N_1^{5/3}}{V_1^{2/3}} \right] = \frac{5}{3} \left(\frac{2\overline{D}}{3} \right)^{2/3} E(N, V, T). \tag{134}$$

ii) Using the low temperature expansion for the energy we obtain to first approximation

$$\frac{12}{5\pi^2(N_1 + N_2)} \left[\frac{N_1^{5/3}}{V_1^{2/3}} + \frac{N_1^{5/3}}{V_1^{2/3}} - \frac{(N_1 + N_2)^{5/3}}{(V_1 + V_2)^{2/3}} \right] \left(\frac{3(N_1 + N_2)}{2\overline{D}(V_1 + V_2)} \right)^{2/3} = (k_B T)^2. \tag{135}$$

iii) They should have the same chemical potential (Fermi energy, concentration of particles), then the divider is virtual and its removal does not lead to a change in the Fermi level and lower degeneracy. The approximate formula (9) shows that in this case, $T = 0$.